# Appendix C, Part 1 Chemical Properties Data

	Chemical	<b>Summary</b>	for	•	•	
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1,3-BENZENEDIOL

1 H-PYRROLE

2-BUTOXYETHANOL ACETATE

2-ETHOXYETHANOL

**AMMONIA** 

**AMMONIUM CHLORIDE** 

**BENZOTRIAZOLE** 

**BORIC ACID** 

**CARBON BLACK** 

COPPER AND SELECTED COPPER COMPOUNDS

DIETHYLENE GLYCOL MONOETHYL ETHER ACETATE

DIETHYLENE GLYCOL METHYL ETHER

DIETHYLENE GLYCOL N-BUTYL ETHER

*N,N*-DIMETHYLFORMAMIDE

**ETHANOLAMINE** 

## CHEMICAL SUMMARY FOR 1,3-BENZENEDIOL

This chemical was identified by one or more suppliers as a bath ingredient for the tin-palladium process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

## I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of 1,3-benzenediol are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF 1,3-BENZENEDIOL

Characteristic/Property	Data	Reference
CAS No.	108-46-3	
Common Synonyms	resorcinol: m-dihydroxybenzene	Budavari et al. 1989
Molecular Formula	$C_6H_6O_2$	Budavari et al. 1989
Chemical Structure		Budavari et al. 1989
	OH	
Physical State	white, needle-like crystals	Budavari et al. 1989
Molecular Weight	110.11	Budavari et al. 1989
Melting Point	109-111°C	Budavari et al. 1989
Boiling Point	280°C	Budavari et al. 1989
Water Solubility	1 g in 0.9 mL	Budavari et al. 1989
Density	1.272	Budavari et al. 1989
Vapor Density (air = 1)	3.79	Keith and Walters 1985
K <sub>oc</sub>	10.36, measured	HSDB 1995
Log K <sub>ow</sub>	0.80, measured	CHEMFATE 1995
Vapor Pressure	2 x 10 <sup>-4</sup> mm Hg @ 25°C	Keith and Walters 1985
Reactivity	hygroscopic; sensitive to light, air; may react with iron	Keith and Walters 1985
	incompatible: acetanilide, albumin, alkalies, antipyrine, camphor, ferric salts, menthol, spirit nitrous ether, urethan	Budavari et al. 1989
Flammability	combustible	Keith and Walters 1985
Flash Point	127.2°C	Keith and Walters 1985
Dissociation Constant	pKa, 9.32, measured	CHEMFATE 1995
	7.11 x 10 <sup>-10</sup> @ 30°C	HSDB 1995
Henry's Law Constant	8.1 x 10 <sup>-11</sup> atm-m <sup>3</sup> /mole @ 25°C	HSDB 1995
Molecular Diffusivity Coefficient	no data	
Air Diffusivity Coefficient	no data	
Fish Bioconcentration Factor	2.4 (estimated)	HSDB 1995
Odor Threshold	faint, characteristic odor	Allan 1994
Conversion Factors	$1 \text{ mg/m}^3 = 0.22 \text{ ppm};$	Calculated using:
	$1 \text{ ppm} = 4.55 \text{ mg/m}^3$	$ppm = 1 \text{ mg/m}^3 \text{ x } 24.45/\text{MW}$

## II. ENVIRONMENTAL FATE

#### A. Environmental Release

1,3-Benzenediol may be released into the environment in waste effluents associated with coal gassification and conversion, coal-tar production, shale oil processing, and from the combustion of wood and tobacco (HSDB 1995). 1,3-Benzenediol is found in cigarette smoke (HSDB 1995). 1,3-

Benzenediol is not one of the chemicals reported to the Toxics Release Inventory (TRI) by certain types of U.S. industries.

## **B.** Transport

1,3-Benzenediol is expected to leach readily in soil; however, leaching may not be important if concurrent biodegradation occurs at a rapid rate (HSDB 1995).

- 1. <u>Air</u> If released to the atmosphere, 1,3-benzenediol can be expected to exist almost entirely in the gas-phase in the ambient atmosphere. Gas-phase 1,3-benzenediol is expected to degrade rapidly in air (estimated half-life 1.9 hours) by reaction with photochemically produced hydroxyl radicals. Night-time reaction with nitrate radicals may also contribute to atmospheric transformation (HSDB 1995).
- 2. <u>Soil</u> 1,3-Benzenediol is readily degradable in soil. The degradation rate decreases at low temperatures (CHEMFATE 1995).
- 3. Water 1,3-Benzenediol is confirmed to be significantly degradable in water (CHEMFATE 1995). By analogy to other phenol compounds, 1,3-benzenediol may react relatively rapidly in sunlit natural water with photochemically produced oxidants such as hydroxyl and peroxyl radicals (HSDB 1995). Hydrolysis, volatilization, and adsorption to sediments are not expected to be important (HSDB 1995).
- 4. <u>Biota</u> Bioconcentration of 1,3-benzenediol is not expected to be important (HSDB 1995).

#### CHEMICAL SUMMARY FOR 1 H-PYRROLE

This chemical was identified by one or more suppliers as a bath ingredient for the conductive polymer process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

#### I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of 1H-pyrrole are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF 1H-PYRROLE

Characteristic/Property	Data	Reference
CAS No.	109-97-7	
Common Synonyms	pyrrole; azole; divinylenimine; imidole	Trochimowicz et al. 1994
Molecular Formula	$C_4H_5N$	Trochimowicz et al. 1994
Chemical Structure	•	
Physical State	liquid (colorless when freshly distilled)	Budavari et al. 1996
Molecular Weight	67.09	Budavari et al. 1996
Melting Point	-23°C	Trochimowicz et al. 1994
Boiling Point	129.8°C @ 760 mm Hg	Budavari et al. 1996
Water Solubility	sparingly soluble	Budavari et al. 1996
Density	specific gravity, 0.9691 <sup>20/4</sup>	Trochimowicz et al. 1994
Vapor Density (air = 1)	2.31	Trochimowicz et al. 1994
K <sub>oc</sub>	not found	
Log K <sub>ow</sub>	0.75 (measured)	Mackay et al. 1995
Vapor Pressure	1100-1136 Pa @ 25°C (8.3-8.5 mm Hg) <sup>a</sup>	Mackay et al. 1995
Reactivity	can react with oxidizing materials; when	HSDB 1996
•	heated to decomposition, emits highly	
	toxic fumes of oxides of nitrogen	
Flammability	must be moderately heated before ignition	HSDB 1996
Ž	occurs	
Flash Point	102°F (390°C)	Budavari et al. 1996
Dissociation Constant	pK <sub>a</sub> , -3.8 to -4.4	Mackay et al. 1995
Henry's Law Constant	1.640 Pa m³/mol (calculated)	Mackay et al. 1995
·	$(1.6 \times 10^{-5} \text{ atm-m}^3/\text{mol})^b$	Ž
Molecular Diffusivity Coefficient	not found	
Air Diffusivity Coefficient	not found	
Fish Bioconcentration Factor	not found	
Odor Threshold	not found	
Conversion Factors	$1 \text{ ppm} = 2.74 \text{ mg/m}^3$	HSDB 1996
	$1 \text{ mg/m}^3 = 0.36 \text{ ppm}$	

a) mm Hg calculated from Pa based on the formula: mm Hg =  $Pa \div 1.333 \times 10^2$  (Lukens 1979).

#### II. ENVIRONMENTAL FATE

#### A. Environmental Release

No information was found in the secondary sources searched regarding the environmental release of 1H-pyrrole. 1H-pyrrole is one of a group of compounds containing five-membered rings with one or more nitrogen atoms (Trochimowicz et al. 1994). The industrial use of the simpler members of this group of chemicals is limited (Trochimowicz et al. 1994). 1H-pyrrole may be released to the environment from plants that manufacture it or use it either as a chemical intermediate in the production of drugs, dyes, herbicides, and perfumes, or as a cross-linking agent for resins (HSDB 1996). However, its limited use would likely preclude the release of large volumes of the chemical to the environment. 1H-pyrrole occurs naturally as part of the

b) Pa converted to atm by the following formula: atm = Pa  $\div$  1.013 x 10 $^{5}$  (Lukens 1979).

structure of pigments such as bilirubin and heme and is a constituent of coal tar and bone oil (Trochimowicz et al. 1994).

## **B.** Transport

No information was found in the secondary sources searched regarding the environmental transport of 1H-pyrrole. The vapor pressure (1100-1136 Pa [Mackay et al. 1995]) and the Henry's Law Constant (1.6 x 10<sup>-5</sup> atm-m³/mol) of the chemical indicate that some volatilization from soil or water could occur. 1H-pyrrole is slightly soluble in water and small amounts may move through the soil, possibly to groundwater.

- 1. <u>Air</u> 1H-pyrrole in air would undergo oxidation, probably within hours. For gas-phase reaction at room temperature the rate constant has been estimated at 1.2 x 10<sup>-10</sup> cm<sup>3</sup> molecule<sup>-1</sup> sec<sup>-1</sup>, assuming the concentration of OH radicals to be 1 x 10<sup>6</sup>/cm<sup>3</sup> during the daytime. This value corresponds to a calculated lifetime of 2.3 hours (Mackay et al. 1995). In other studies, the calculated lifetime was 1.4 minutes for reaction with NO<sub>3</sub> radicals during nighttime hours and 24 hours for reaction with O<sub>3</sub> molecules (Mackay et al. 1995).
- 2. <u>Soil</u> No information was found in the secondary sources searched regarding the degradation of 1H-pyrrole in the soil.
- 3. <u>Water</u> No information was found in the secondary sources searched regarding the degradation of 1H-pyrrole in water.
- 4. <u>Biota</u> The log K<sub>OW</sub> for 1H-pyrrole (0.75 [Mackay et al. 1995]) indicates that the chemical has a low to moderate potential to bioaccumulate in aquatic organisms.

#### CHEMICAL SUMMARY FOR 2-BUTOXYETHANOL ACETATE

This chemical was identified by one or more suppliers as a bath ingredient for the conductive ink process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online data bases, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

#### I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of 2-butoxyethanol acetate are listed below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF 2-BUTOXYETHANOL ACETATE

Characteristic/Property	Data	Reference
CAS No.	112-07-2	
Common Synonyms	ethylene glycol monobutyl ether acetate;	
• •	Butyl Cellosolve acetate	HSDB 1996
Molecular Formula	$C_8H_{16}H_3$	Gingell et al. 1994
Chemical Structure	$C_4H_9$ -O-(CH <sub>2</sub> ) <sub>2</sub> -OCOCH <sub>3</sub>	NIOSH 1994
Physical State	colorless liquid	HSDB 1996
Molecular Weight	160.21	Gingell et al. 1994
Melting Point	-64.5°C	Howard 1993
Boiling Point	192.3°C	Howard 1993
Water Solubility	15,000 mg/L at 20°C	Verschueren 1996
Density	0.9422 @ 20/20°C	HSDB 1996
Vapor Density (air = 1)	5.5	HSDB 1996
K <sub>oc</sub>	26 (calculated)	HSDB 1996
Log K <sub>ow</sub>	1.51 (measured)	Verschueren 1996
Vapor Pressure	0.375 mm Hg @ 20°C	Howard 1993
Reactivity	can react with oxidizers	NIOSH 1994
Flammability	NFPA rating $= 2$ ; must be moderately	
•	heated before ignition can occur	HSDB 1996
Flash Point	71 °C (160 °F) (closed cup)	HSDB 1996
Dissociation Constant	no data	
Air Diffusivity Constant	no data	
Molecular Diffusivity Constant	no data	
Henry's Law Constant	$7.19 \times 10^{-6} \text{ atm-m}^{3}/\text{mole}$	Howard 1993
Fish Bioconcentration Factor	3.2 (calculated)	Howard 1993
Odor Threshold	0.10 ppm, abs. perception limit;	
	0.35 ppm, 50% recognition;	
	0.48 ppm, 100% recognition	Verschueren 1996
Conversion Factors	$1 \text{ ppm} = 6.64 \text{ mg/m}^3$	
	$1 \text{ mg/m}^3 = 0.15 \text{ ppm}$	Verschueren 1996

## II. ENVIRONMENTAL FATE

#### A. Environmental Release

2-Butoxyethanol acetate may be released to the atmosphere by evaporation when it is used as a solvent in paints, lacquers, thinners, inks, and resins. The emission rate into the atmosphere from painting operations in an automobile assembly plant in Wisconsin was estimated at 37.9 gallons/hour (Howard 1993). 2-Butoxyethanol acetate was detected in 0.4% of 275 solvent products that were sampled in various industries and analyzed between 1978 and 1982 (HSDB 1996).

In 1993, releases of all glycol ethers to environmental media, as reported in the TRI by certain types of industries, totaled about 45.9 million pounds; 2-butoxyethanol acetate is not listed separately (TRI93 1995).

#### **B.** Transport

The estimated relatively low  $K_{\rm OC}$  of 26 suggests that 2-butoxyethanol acetate can leach readily into groundwater from soils. However, if rapid biodegradation occurs, leaching may be less important. Volatilization from water is expected to be slow, with the possible exception from very shallow rivers. Physical removal via wet deposition is likely because the chemical is soluble in water (Howard 1993; HSDB 1996).

- 1. <u>Air</u> Based on a vapor pressure of 0.375 mm Hg at 20°C, 2-butoxyethanol acetate should exist almost entirely in the vapor phase in the atmosphere. It is expected that 2-butoxyethanol acetate will degrade by reaction with hydroxyl radicals with an estimated half-life of about 18.4 hours (HSDB 1996).
- 2. <u>Soil</u> When released to soils, biodegradation is expected to be the most important removal process. One biodegradation screening study demonstrated that the chemical is readily (>90%) biodegraded (HSDB 1996).
- 3. Water Biodegradation is likely to be the most important removal mechanism of 2-butoxyethanol acetate from aquatic systems. In a screening assay, 2-butoxyethanol acetate total degradation exceeded 90%, with a measured rate of 12%/day under the test conditions. No observable lag period was required before onset of degradation. Estimated volatilization half-lives from a model river (1 meter deep) and model pond are 6.6 and 74 days, respectively. Adsorption to sediment is not expected to be important (HSDB 1996).
- 4. <u>Biota</u> The estimated bioconcentration factor of 3.2 suggests that 2-butoxyethanol acetate would not bioconcentrate significantly in aquatic organisms (Howard 1993).

#### CHEMICAL SUMMARY FOR 2-ETHOXYETHANOL

This chemical was identified by one or more suppliers as a bath ingredient for the electroless copper process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

## I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of 2-ethoxyethanol are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF 2-ETHOXYETHANOL

Characteristic/Property	Data	Reference
CAS No.	110-80-5	
Common Synonyms	ethylene glycol monoethyl ether;	
• •	Cellusolve; Oxitol	Budavari et al. 1996
Molecular Formula	$C_4H_{10}O_2$	Budavari et al. 1996
Chemical Structure	HOCH,CH,OC,H,	Budavari et al. 1996
Physical State	colorless liquid	Budavari et al. 1996
Molecular Weight	90.12	Budavari et al. 1996
Melting Point	-70°C	Budavari et al. 1996
Boiling Point	135°C	Budavari et al. 1996
Water Solubility	miscible	Budavari et al. 1996
·	$\geq 100 \text{ mg/mL}$	Keith and Walters 1985
Density	0.93	Budavari et al. 1996
Vapor Density (air = 1)	3.10	Verschueren 1996
Koc	0.12 (calculated)	Howard 1990
Log K <sub>ow</sub>	-0.10	Howard 1990
Vapor Pressure	3.8 mm Hg at 20°C	Verschueren 1996
Reactivity	reacts with strong oxidizers	Keith and Walters 1985
Flammability	combustible	Keith and Walters 1985
Flash Point	44°C (closed cup)	Budavari et al. 1996
	49°C (open cup)	
Dissociation Constant	no data	
Henry's Law Constant	$5.13 \times 10^{-2} \text{ atm-m}^3/\text{mol}$	Howard 1990
Molecular Diffusivity Coefficient	no data	
Air Diffusivity Coefficient	no data	
Fish Bioconcentration Factor	no data	
Odor Threshold	0.55 ppm (50% recognition)	Verschueren 1996
	1.33 ppm (100% recognition)	Verschueren 1996
Conversion Factors	1 ppm = $3.75 \text{ mg/m}^3$	Verschueren 1996
	$1 \text{ mg/m}^3 = 0.27 \text{ ppm}$	

## II. ENVIRONMENTAL FATE

#### A. Environmental Release

Environmental release of 2-ethoxyethanol can occur from wastewater effluents and atmospheric emissions from production and use facilities. Information on the amount of 2-ethoxyethanol released to the environment was not found in the secondary sources searched. Chemical concentrations detected in the Hayashida River (Japan) were 250-1200 ppb (Howard 1990; U.S. EPA 1985a). Effluent from a facility in Brandenburg, KY contained 0.10  $\mu$ g/L in 1974 (U.S. EPA 1985a).

#### **B.** Transport

The Henry's Law constant of  $5.13 \times 10^{-2}$  atm-m³/mol (Howard 1990) indicates rapid volatilization from soils and surface waters. The complete water solubility and low  $K_{OC}$  indicate that leaching from soils into ground water may occur.

- 1. <u>Air</u> In the atmosphere, 2-ethoxyethanol will react with both nitrogen oxides and hydroxyl radicals. The half-life of the chemical was 9.8 hour when mixed with nitrogen oxides (20:1, 2-ethoxyethanol:nitrogen dioxides) in a smog chamber. For reaction with photochemically produced hydroxy radicals, the estimated half-life is 11.41 hours (Howard 1990).
- 2. Soil Volatilization and biodegradation are the main removal mechanisms for 2-ethoxyethanol from soils. Adsorption is not expected to be significant, so leaching into ground waters may occur (Howard 1990). A soil microbe acclimated to triethylene glycol was capable of utilizing 2-ethoxyethanol as a sole carbon source. In a standard evaporation test at 77°C and 15% relative humidity, 100% loss of the chemical occurred in 20 minutes (U.S. EPA 1985a).
- 3. Water 2-Ethoxyethanol will volatilize readily from surface waters with biodegradation also contributing to removal. After incubation of the chemical for 5 days with either sewage seed or activated sludge, 7.6% and up to 65%, respectively, of the theoretical biological oxygen demand was achieved. Adsorption to suspended particulates and sediments is not expected to occur (Howard 1990). Hydrolysis of 2-ethoxyethanol is not expected to be important (U.S. EPA 1985a).
- 4. <u>Biota</u> Based on the complete water solubility and low K<sub>ow</sub> of 2-ethoxyethanol, the chemical is not expected to accumulate in aquatic organisms (U.S. EPA 1985a).

## CHEMICAL SUMMARY FOR AMMONIA

This chemical was identified by one or more suppliers as a bath ingredient for the graphite process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

## I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of ammonia are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF AMMONIA

Characteristic/Property	Data	Reference
CAS No.	7664-41-7	
Common Synonyms	ammonia gas; liquid ammonia; ammonia,	
•	anhydrous; Spirit of Hartshorn; Nitro-Sil	Lockheed Martin 1995a
Molecular Formula	$H_3N$	
Chemical Structure	•	
	H— $N$ — $H$	
	Н	
Physical State	colorless gas	Budavari et al. 1989
Molecular Weight	17.03	Budavari et al. 1989
Melting Point	-77.7°C	Budavari et al. 1989
Boiling Point	-33.35°C	Budavari et al. 1989
Water Solubility	47% @ 0°C; 38% @ 15°C; 34% @ 20°C	Budavari et al. 1989
Density	0.7710 g/L (gas)	ATSDR 1990a
Vapor Density (air = 1)	0.59	HSDB 1995
K <sub>oc</sub>	no data	
Log K <sub>ow</sub>	no data	
Vapor Pressure	$7.508 \times 10^{3} \text{ mm Hg } @ 25^{\circ}\text{C}$	CHEMFATE 1995
Reactivity	incompatible with halogens, acid chlorides,	
•	acid, acid anhydrides, oxidizing agents,	
	chloroformates, galvanized iron; reacts	
	with zinc, copper, tin, and their alloys;	Lockheed Martin 1995a
	pH of 1N solution = 11.6	Budavari et al. 1989
Flammability	flammable	
Flash Point	no data; autoignition @ 649°C	Lockheed Martin 1995a
Dissociation Constant	$pKa = 9.249$ ; $pKb = 4.751 @ 25^{\circ}C$	U.S. EPA 1981a
Henry's Law Constant	$7.3 \times 10^{-6}$ atm-m <sup>3</sup> /mole (pH 7, 23.4°C)	
•	$1.6 \times 10^{-5} \text{ atm-m}^3/\text{mole } (25^{\circ}\text{C})$	ATSDR 1990a
Molecular Diffusivity Coefficient	no data	
Air Diffusivity Coefficient	no data	
Fish Bioconcentration Factor	no data	
Odor Threshold	1.5 ppm (water); 25 ppm (air)	ATSDR 1990a
Conversion Factors	$1 \text{ ppm} = 0.708 \text{ mg/m}^3$	
	$1 \text{ mg/m}^3 = 1.41 \text{ ppm}$	ATSDR 1990a

#### II. ENVIRONMENTAL FATE

#### A. Environmental Release

Ammonia is an important component of the nitrogen cycle such that concentrations in nature and natural media are in dynamic equilibrium (ATSDR 1990a). Natural sources of ammonia include volcanic eruptions, forest fires, microbial fixation of nitrogen, microbial decomposition of dead plants and animals, and decay of livestock, pet, and human wastes (ATSDR 1990a). Approximately 80% of the ammonia produced in the U.S. is applied to soils as fertilizer (ATSDR 1990a).

Average concentrations have been measured at <0.18 mg/L in surface waters and approximately 0.5 mg/L in waters near metropolitan areas; concentrations were lower in the summer than in the winter (U.S. EPA 1981a). Average global atmospheric ammonia concentrations are 1-3 ppb (ATSDR 1990a).

In 1993, as reported to the TRI, a total of 353 million pounds of ammonia were released to the environment. Of the total, 138 million pounds were released to the atmosphere, 36 million pounds were released surface waters, 169 million pounds were released to underground injection sites, and 10 million pounds were released to land (TRI93 1995).

### **B.** Transport

As a key component of the nitrogen cycle, ammonia in water and soils undergoes microbial mediated nitrification. The resulting nitrates are assimilated into plants and other microbes. This process is dependent upon dissolved oxygen, temperature, pH, the microbial population, and the nitrogen forms present (U.S. EPA 1981a; ATSDR 1990a). From natural waters, ammonia also volatilizes to the atmosphere or strongly adsorbs to sediment so that leaching is not likely (U.S. EPA 1981a). Once in the atmosphere, the chemical can be removed in rain or snow or dissolve in clouds (ATSDR 1990a).

- Air In the atmosphere, ammonia reacts with acid air pollutants such as HNO<sub>3</sub> and H<sub>2</sub>SO<sub>4</sub> to form particulate ammonium compounds that can be removed by wet or dry deposition (ATSDR 1990a). In unpolluted air, the half-life for ammonia reaction with hydroxyl radicals is about 16 days (U.S. EPA 1981a).
- Soil In soils, ammonia is transformed to nitrate by soil microbes and taken up by plants as a
  nutrient source. The ammonium cation adsorbs to negatively charged clay colloids in soils and
  is relatively immobile. Volatilization is another removal mechanism from soil (ATSDR 1990a;
  U.S. EPA 1981a).
- 3. <u>Water</u> In natural waters, ammonia undergoes nitrification with the products being taken up by aquatic plants or other organisms. Ammonia can also adsorb to sediments or volatilize to the atmosphere (ATSDR 1990a; U.S. EPA 1981a).
- 4. <u>Biota</u> Ammonia is a natural waste product of fish and is released to the surrounding water through the gills. If water concentrations are abnormally high, the concentration gradient is reversed and the direction of passive transport is into the gills (ATSDR 1990a).

#### CHEMICAL SUMMARY FOR AMMONIUM CHLORIDE

This chemical was identified by one or more suppliers as a bath ingredient for the electroless copper process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

#### I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of ammonium chloride are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF AMMONIUM CHLORIDE

Characteristic/Property	Data	Reference
CAS No.	12125-02-9	
Common Synonyms	ammonium muriate; sal ammoniac	Sax and Lewis 1989
Molecular Formula	ClH₄N	Budavari et al. 1989
Chemical Structure	H <sub>4</sub> N-Cl	
Physical State	white crystalline solid, somewhat	
•	hygroscopic	ACGIH 1991
Molecular Weight	53.50	Budavari et al. 1989
Melting Point	sublimes @ 350°C without melting	ACGIH 1991
Boiling Point	520°C	Sax and Lewis 1989
Water Solubility	28.3% (w/w) @ 25°C	Budavari et al. 1989
Density	1.5274 at 25°C	Budavari et al. 1989
Vapor Density (air = 1)	no data	
K <sub>oc</sub>	no data	
Log K <sub>ow</sub>	no data	
Vapor Pressure	1 mm Hg @ 160.4°C	Sax and Lewis 1989
Reactivity	reacts with alkalis & their carbonates;	
	lead & silver salts; strong oxidizers;	
	ammonium nitrate; potassium chlorate; and	
	bromine trifluoride; corrodes most metals	NIOSH 1994
Flammability	not flammable	HSDB 1995
Flash Point	no data	
Dissociation Constant	no data	
Henry's Law Constant	no data	
Molecular Diffusivity Coefficient	no data	
Air Diffusivity Coefficient	no data	
Fish Bioconcentration Factor	no data	
Odor Threshold	odorless	Budavari et al. 1989
Conversion Factors	no data	

#### II. ENVIRONMENTAL FATE

## A. Environmental Release

Ammonium chloride, a somewhat hygroscopic crystalline solid with a cooling saline taste, is highly soluble in water (Budavari et al. 1989). It is used in dry batteries; soldering; manufacture of various ammonia compounds; as a fertilizer; in electroplating; in medicine; and in the food industry (ACGIH 1991; Verschueren 1983). Large amounts of ammonium chloride are frequently evolved from galvanizing operations, with concentrations generally below 5 mg/m³, although peak concentrations are higher (ACGIH 1991). Ammonium chloride occurs naturally in crevices in the vicinity of volcanoes (Young 1978).

## **B.** Transport

No information on the transport of ammonium chloride was found in the secondary sources searched. The water solubility suggests that the chemical would leach through soil.

## C. Transformation/Persistence

No information on the transformation/persistence of ammonium chloride was found in the secondary sources searched. Low vapor pressure and its water solubility suggest the chemical would remain in the aqueous phase.

#### CHEMICAL SUMMARY FOR BENZOTRIAZOLE

This chemical was identified by one or more suppliers as a bath ingredient for the electroless copper process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

#### I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of benzotriazole are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF BENZOTRIAZOLE

Characteristic/Property	Data	Reference
CAS No.	95-14-7	
Common Synonyms	1,2,3-benzotriazole; 1H-benzotriazole; azimino-	RTECS 1995
	benzene; 1,2-aminozophenylene; benzene azimide	
Molecular Formula	$C_6H_5N_3$	
Chemical Structure		
Physical State	white to light tan crystalline powder	HSDB 1995
Molecular Weight	119.14	RTECS 1995
Melting Point	98.5°C	HSDB 1995
Boiling Point	204°C @ 15 mm Hg	HSDB 1995
Water Solubility	19.8 g/L @ 25°C (measured)	CHEMFATE 1995
Density	not found	
Vapor Density (air = 1)	not found	
K <sub>oc</sub>	not found	
Log K <sub>ow</sub>	1.34 (measured)	CHEMFATE 1995
Vapor Pressure	0.4 x 10 <sup>-1</sup> Torr @ 20°C (measured)	CHEMFATE 1995
Reactivity	stable toward acids, alkalies, oxidation and	HSDB 1995
	reduction; forms stable metallic salts; may	
	explode during vacuum distillation	
Flammability	1.6 @ 20°C (measured)	CHEMFATE 1995
Flash Point	not found	
Dissociation Constant	not found	
Henry's Law Constant	not found	
Molecular Diffusivity Coefficient	not found	
Air Diffusivity Coefficient	not found	
Fish Bioconcentration Factor	not found	
Odor Threshold	not found	
Conversion Factors	$1 \text{ ppm} = 4.87 \text{ mg/m}^3$	Calculated using:
	$1 \text{ mg/m}^3 = 0.205 \text{ ppm}$	$ppm = mg/m^3 \times 24.45/m.w$

#### II. ENVIRONMENTAL FATE

#### A. Environmental Release

Benzotriazole may be released to the environment during its production and its use in a wide range of commercial products. Uses of the chemical include: as a chemical intermediate; as a pickling inhibitor in boiler scale removal; as a restrainer, developer and antifogging agent in photographic emulsions; as a corrosion inhibitor for copper; as a component of military deicing fluid; and as a plastics stabilizer (HSDB 1995). The NCI (1977) selected the chemical for study in the bioassay program because of its use in dishwashing detergents and the possibility that such use could result in the contamination of water supplies.

### **B.** Transport

The considerable water solubility of benzotriazole (19.8 g/L [CHEMFATE 1995]) suggests that the chemical may exist in solution in the soil and leach into ground water. The low vapor pressure (0.04 Torr at 20°C [CHEMFATE 1995]) indicates that volatilization is not a significant transport

mechanism for benzotriazole in soil or water. In one instance, benzotriazole evaporated from water in 438 hours (~18 days) (CHEMFATE 1995). Because of its water solubility, benzotriazole present in the atmosphere may be removed by wet deposition.

- <u>Air</u> No information was found in the secondary sources searched regarding the transformation/persistence of benzotriazole in air. The considerable water solubility of benzotriazole (see section II.B) suggests that the chemical would be removed from the atmosphere by wet deposition.
- 2. Soil The sensitivity of benzotriazole to photodegradation is solvent-dependent (CHEMFATE 1995). The chemical was 100% degraded when irradiated for 60 hours at 300 nm in methanol (CHEMFATE 1995). The products of degradation (also solvent-dependent) were aniline (1-1.6%) and *O*-anisidine (2-8.2%).
- 3. Water In one study, benzotriazole as the sole source of carbon was not degraded by acclimated sludge in water (CHEMFATE 1995). Other investigators observed that elective cultures and continuous enrichment failed to biodegrade benzotriazole and indicated that the chemical is expected to resist degradation in the environment (Rollinson and Callely 1986). In the aquatic environment, the chemical could undergo some photolysis at the water's surface (see section II.C.2).
- 4. <u>Biota</u> The log octanol/water partition coefficient for benzotriazole, 1.34 (CHEMFATE 1995), suggests that the chemical has a low to moderate potential for partitioning to lipids. However, no information was found to indicate whether the chemical will bioaccumulate.

#### CHEMICAL SUMMARY FOR BORIC ACID

This chemical was identified by one or more suppliers as a bath ingredient for the electroless copper process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

## I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of boric acid are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF BORIC ACID

Characteristic/Property	Data	Reference
CAS No.	10043-35-3	
Common Synonyms	boracic acid	Budavari et al. 1989
• •	orthoboric acid	HSDB 1995
Molecular Formula	$H_3BO_3$	
Chemical Structure		
Physical State	colorless, odorless, transparent crystals; or white granules or powder	Budavari et al. 1989
Molecular Weight	61.84	Budavari et al. 1989
Melting Point	171°C	Budavari et al. 1989
Boiling Point	300°C	U.S. EPA 1990a
Water Solubility	1 g/18 ml cold H <sub>2</sub> O	Budavari et al. 1989
Density	1.435 @ 15°C	U.S. EPA 1990a
Vapor Density (air = 1)	no data	
K <sub>oc</sub>	no data	
Log K <sub>ow</sub>	no data	
Vapor Pressure	low for boron compounds	U.S. EPA 1990
Reactivity	incompatible with alkali carbonates and hydroxides	Budavari et al. 1989
	mixtures with potassium may explode on impact	HSDB 1995
Flammability	not flammable	HSDB 1995
Flash Point	not flammable	HSDB 1995
Dissociation Constant	no data	
Henry's Law Constant	no data	
Molecular Diffusivity Coefficient	no data	
Air Diffusivity Coefficient	no data	
Fish Bioconcentration Factor	no data	
Odor Threshold	odorless	Budavari et al. 1989
Conversion Factors	no data	

#### II. ENVIRONMENTAL FATE

#### A. Environmental Release

Boric acid is a naturally occurring compound formed from the breaks of other boron compounds. It is released into the atmosphere during volcanic eruptions; however, most of this is captured by the oceans. Boric acid also enters the environment as a contaminant from the manufacture and industrial and household use of boron-containing compounds; the mining and processing of borax; coal, oil and geothermal power generation; and sewage and sludge disposal (U.S. EPA 1990a). Boric acid is not listed on the EPA's TRI, requiring certain types of U.S. industries to report on chemical releases to the environment.

#### **B.** Transport

Groundwater movement studies indicate that boron is relatively mobile in sand and gravel aquifers, with retardation only occurring as a result of adsorption to clay or organic materials. An equilibrium exists between adsorbed and dissolved boron in soils (U.S. EPA 1990a).

- 1. <u>Air</u> Boron does not appear to persist in the atmosphere as a vapor. As a particulate, boron can be removed by either wet or dry deposition (U.S. EPA 1990a).
- 2. <u>Soil</u> Boric acid is adsorbed onto soil at acidic pH levels, and does not appear to be chemically or biologically degraded in soils (U.S. EPA 1990a).
- 3. <u>Water</u> In natural waters, boron does not appear to be chemically or biologically degraded, but exists as undissociated boric acid (U.S. EPA 1990a). Because of its low vapor pressure, volatilization is not expected to be a contributing factor for the release of boron at the air-water interface (U.S. EPA 1990a).
- 4. <u>Biota</u> No specific information was found in the secondary sources searched regarding the bioaccumulation of boric acid. However, boron accumulation appears to occur in relation to its availability in the surrounding aquatic systems. Tissue concentrations of boron in fish from freshwater aquatic systems of varying water quality containing boron or boron compounds (not necessarily just boric acid) have been reported to range from  $1.8 \mu g/g$  in lake charr from a Precambrian shield lake to  $20 \mu g/g$  in carp from a river system receiving agricultural subsurface drainage (U.S. EPA 1990a).

#### CHEMICAL SUMMARY FOR CARBON BLACK

This chemical was identified by one or more suppliers as a bath ingredient for the carbon and conductive ink processes. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

## I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of carbon black are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF CARBON BLACK

Characteristic/Property	Property Data		
CAS No.	1333-86-4		
Common Synonyms	lamp black; thermal black; furnace black;	HSDB 1996	
	acetylene black; channel black; CI pigment		
	black 7; philblack N 550; raven; regal;		
M. I. F. I.	carbon, amorphous		
Molecular Formula	C	H.G. EDA 10011	
Chemical Structure	microscopic hexagonal crystallites oriented randomly	U.S. EPA 1981b	
Physical State	extremely fine, smoke-like powder; black	HSDB 1996	
Molecular Weight	12; may vary with manufacturing process	NIOSH 1994; U.S. EPA 1981b	
Melting Point	sublimates @ 3652-3697°C	HSDB 1996	
Boiling Point	4200°C; 4827°C	HSDB 1996;	
		U.S. EPA 1981b	
Water Solubility	insoluble	<b>U.S.</b> EPA 1981b	
Density	1.8-2.1	U.S. EPA 1981b	
Vapor Density $(air = 1)$	not applicable		
K <sub>oc</sub>	not found		
Log K <sub>ow</sub>	not found		
Vapor Pressure	0 mm Hg (approximately)	NIOSH 1994	
Reactivity	reacts with strong oxidizers, such as	NIOSH 1994; HSDB 1996	
	chlorates, bromates and nitrates; carbon		
	dust may form explosive mixtures in air		
Flammability	flammable	HSDB 1996	
Flash Point	not found		
Dissociation Constant	not found		
Henry's Law Constant	not found		
Molecular Diffusivity Coefficient	not found		
Air Diffusivity Coefficient	not found		
Fish Bioconcentration Factor	not found		
Odor Threshold	odorless	HSDB 1996	
Conversion Factors	not applicable		

Analytical properties of commercially produced carbon blacks (all with CAS No. 1333-86-4) are summarized below. Contaminants, including polynuclear aromatic hydrocarbons (PAHs), adsorb to carbon-black particles (IARC 1984). These contaminants (some are known carcinogens) are extractable with organic solvents such as benzene, naphthalene, and toluene (IARC 1984). The efficiency of the extraction depends on the solvent, extraction time, type of carbon black, relationship between sample weight/solvent volume and the amount of extractable material. The bioavailability of these potential carcinogens is an important issue in the assessment of the health effects of carbon black (IARC 1984). Available evidence indicates that when carbon blacks are exposed to biological material, including human albumin, some release of PAHs occurs, depending on the amount of adsorbed material and the available adsorptive surface (IARC 1984).

Property	nalytical Data for Carbon Blacks Produced Con Channel Acetylene Furnace	Lampblack	Thermal			
	Black <sup>a</sup>	-		_	Medium	Fine
Average particle diameter (nm)	29	40	28	65	500	180
Benzene extract (%)		0.1	0.06	0.2	0.3	0.8
pH	acidic	4.8	7.5	3.0	8.5	9.0
Volatile material (%)	5-17%	0.3	1.0	1.5	0.5	0.5
Composition (%)						
Carbon		99.7	97.9	98	99.3	99.2
Hydrogen		0.1	0.4	0.2	0.3	0.5
Sulfur		0.02	0.6	0.8	0.01	0.01
Oxygen		0.2	0.7	0.8	0.1	0.3

a) No longer produced in the U.S. Certain carbon blacks made in Germany by an impingement process reportedly have the same properties as the old channel black (IARC 1984). Only general properties were available for channel black.

Source: IARC (1984)

#### II. ENVIRONMENTAL FATE

#### A. Environmental Release

Carbon black may be released to the environment from various production facilities and from rubber tires in which carbon black is used as a reinforcing agent (U.S. EPA 1981b). The objective of the carbon-black industry is to produce large quantities of dense carbon smoke that would, under ordinary circumstances, be considered an undesired by-product (U.S. EPA 1981b). Consequently, for economic reasons, releases from production facilities are limited by highly efficient collection methods. In the thermal and furnace process plants, systems of electrostatic precipitators, cyclones, and bag filters collect over 99% of the black (U.S. EPA 1981b). In the channel production process (no longer used in the U.S.), carbon black was collected by a less effective method, impingement on long-channel irons, and larger quantities of carbon black were released (U.S. EPA 1981b). Releases to the atmosphere may also occur during maintenance procedures, from leaks in plant conveying systems, or during loading and unloading operations (U.S. EPA 1981b). In 1979, average particulate carbon-black emissions during the manufacture of carbon blacks by the oil furnace process ranged from 0.1 kg/thousand kg for fugitive emissions to 3.27 kg/thousand kg from uncontrolled main process vents (IARC 1984). More recent monitoring data were not found in the secondary sources searched.

As a result of tire wear, carbon black is deposited in significant quantities along roadways, apparently settling out within a few feet of the road (U.S. EPA 1981b).

In 1978, the U.S. EPA issued its final regulation on water discharge permits that called for zero discharge of carbon black using the best available technology (U.S. EPA 1981b).

#### **B.** Transport

Carbon black entering the atmosphere or lost from tires ultimately enters the soil or is washed into the waterways (U.S. EPA 1981b). No other information was found in the secondary sources searched regarding environmental transport of carbon black.

#### C. Transformation/Persistence

No information was found in the secondary sources searched regarding the transformation/persistence of carbon black in the atmospheric, aquatic, or terrestrial environment or in biota. It is expected to be inert under normal conditions (U.S. EPA 1981b).

## CHEMICAL SUMMARY FOR COPPER AND SELECTED COPPER COMPOUNDS

These chemicals were identified by one or more suppliers as bath ingredients for the electroless copper, carbon, graphite, non-formaldehyde electroless copper, and tin-palladium processes. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

## I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of copper, cupric sulfate, cuprous chloride, cupric chloride, and cupric ethylenediaminetetraacetate (Cu-EDTA) are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF COPPER

Characteristic/Property	Data	Reference			
CAS No.	7440-50-8				
Common Synonyms	None				
Molecular Formula	Cu				
Chemical Structure	$\mathrm{Cu}^0$				
Physical State	Reddish metal	U.S. EPA 1987a			
Molecular Weight	63.55	U.S. EPA 1987a			
Melting Point	1083.4°C	U.S. EPA 1987a			
Boiling Point	2567°C	U.S. EPA 1987a			
Water Solubility	Insoluble (as Cu°)	U.S. EPA 1987a			
Specific Gravity	8.92	U.S. EPA 1987a			
Vapor Density (air = 1)	No data				
K <sub>oc</sub>	No data				
Log K <sub>ow</sub>	No data				
Vapor Pressure	1 mm Hg @ 1629°C	U.S. EPA 1987a			
Reactivity	Reacts with dil. HNO <sub>3</sub> , conc. H <sub>2</sub> SO <sub>4</sub> , and organic acids;	Budavari et al. 1989			
•	slowly with HCl in the presence of oxygen. Forms	U.S. Air Force 1990			
	carbonate salt on the metal surface in moist air.	HSDB 1995			
	Forms soluble salts on the metal surface in water.				
	Violent reaction with hydrazoic acid, hydrogen				
	sulfide, lead azide, sodium azide, hydrazine mono-				
	nitrate, ammonium nitrate, bromates, chlorates,				
	iodates, chlorine, fluorine, and peroxides. Can react				
	with acetylene to form explosive acetylides.				
Flammability	No data				
Flash Point	No data				
Dissociation Constant	No data				
Henry's Law Constant	No data				
Molecular Diffusivity Coefficient	No data				
Air Diffusivity Coefficient	No data				
Fish Bioconcentration Factor	10-100	ATSDR 1990b			
Shellfish Bioconcentration Factor	30,000 in oysters ATSDR 1990b				
Taste Threshold (copper in water)	2.6 ppm ATSDR 1990b				
Conversion Factors	Not applicable, associated with particulate matter				

## APPENDIX C

## CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF CUPRIC SULFATE

Characteristic/Property	Data	Reference
CAS No.	7758-98-7	
Common Synonyms	Copper Sulfate; Blue Vitriol	ATSDR 1990b
Molecular Formula	$CuSO_4$	ATSDR 1990b
Chemical Structure	$CuO_4S$	ATSDR 1990b
Physical State	Solid, White powder (anhydrous),	ATSDR 1990b
	blue crystals (hydrated)	
Molecular Weight	159.60 (dehydrated)	ATSDR 1990b
	249.68 (pentahydrate)	U.S. EPA 1987a
Melting Point	Decomposes @ 110°C	U.S. EPA 1987a
Boiling Point	Decomposes to CuO @ 650°C	ATSDR 1990b
Water Solubility	143 g/L @ 0°C	ATSDR 1990b
Specific Gravity	3.603 (anhydrous)	ATSDR 1990b
	2.284 (pentahydrate)	U.S. EPA 1987a
Vapor Density (air = 1)	No data	
$K_{OC}$	No data	
Log K <sub>ow</sub>	No data	
Vapor Pressure	No data	
Reactivity	Reacts with Mg to produce Cu <sub>2</sub> O, MgSO <sub>4</sub> , and H <sub>2</sub> ;	U.S. Air Force 1990
	reacts with NH <sub>4</sub> Cl producing (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> and CuCl <sub>2</sub> ;	HSDB 1995
	reacts with alkali (R)OH to produce Cu(OH)2 and RSO	
	reacts with excess aq. NH <sub>3</sub> producing Cu(NH <sub>3</sub> ) <sub>2</sub> <sup>++</sup> + OI	₫ <sup>-</sup> ;
	decomposition products include SO <sub>2</sub> .	
Flammability	Non-flammable	HSDB 1995
Flash Point	Non-flammable	HSDB 1995
Dissociation Constant	No data	
Henry's Law Constant	No data	
Molecular Diffusivity Coefficient	No data	
Air Diffusivity Coefficient	No data	
Fish Bioconcentration Factor	10-100 for copper	ATSDR 1990b
Shellfish Bioconcentration Factor	30,000 for copper in oysters	ATSDR 1990b
Taste Threshold (copper in water)	2.6 ppm for copper	ATSDR 1990b
Conversion Factors	Not applicable, associated with particulate material	

## CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF CUPROUS CHLORIDE

Characteristic/Property	Data	Reference
CAS No.	7758-89-6	
Common Synonyms	Copper (I) chloride	U.S. EPA 1987a
Molecular Formula	CuCl	U.S. EPA 1987a
Chemical Structure	CuCl (or Cu <sub>2</sub> Cl <sub>2</sub> )	U.S. EPA 1987a
Physical State	Solid, White crystal	U.S. EPA 1987a
Molecular Weight	98.99	U.S. EPA 1987a
Melting Point	430°C	U.S. EPA 1987a
Boiling Point	1490°C	U.S. EPA 1987a
Water Solubility	0.062 g/L (cold water)	U.S. EPA 1987a
Specific Gravity	4.14	U.S. EPA 1987a
Vapor Density (air = 1)	No data	
K <sub>oc</sub>	No data	
$\text{Log } K_{\text{OW}}$	No data	
Vapor Pressure	1 mm Hg @ 546°C	U.S. EPA 1987a
Reactivity	Reactive with oxidizing agents, alkali metals;	Aldrich Chemical Co. 1985
	decomposition products include HCL gas.	
Flammability	Not combustible	
Flash Point	Not combustible	
Dissociation Constant	No data	
Henry's Law Constant	No data	
Molecular Diffusivity Coefficient	No data	
Air Diffusivity Coefficient	No data	
Fish Bioconcentration Factor	10-100 for copper	ATSDR 1990b
Shellfish Bioconcentration Factor	30,000 for copper in oysters	ATSDR 1990b
Taste Threshold (copper in water)	2.6 ppm	ATSDR 1990b
Conversion Factors	Not applicable, associated with particulate material	

CHEMICAL IDEN	TITY AND C	HEMICAI /DHVSICA	I DDODEDTIES OF	CUPRIC CHLORIDE
CHEWIICAL IDEN	IIIIX AND C	OEWIICAL/PO ISICA	L PROPERTIES OF	CUPRIC CHLORIDE

Characteristic/Property	Data	Reference
CAS No.	7447-39-4	
Common Synonyms	Copper (II) chloride	U.S. EPA 1987a
Molecular Formula	$CuCl_2$	U.S. EPA 1987a
Chemical Structure	$CuCl_2$	U.S. EPA 1987a
Physical State	Brown or yellow powder	U.S. EPA 1987a
	Green to blue crystals when hydrated	EM Industries 1987
Molecular Weight	134.44	U.S. EPA 1987a
Melting Point	620°C	U.S. EPA 1987a
Boiling Point	Decomposes @ 993°C	U.S. EPA 1987a
Water Solubility	706 g/L @ 0°C	U.S. EPA 1987a
Specific Gravity	$3.386^{4/25}$	U.S. EPA 1987a
Vapor Density (air = 1)	No data	
K <sub>oc</sub>	No data	
Log K <sub>ow</sub>	No data	
Vapor Pressure	No data	
Reactivity	HCl gas can be produced in fires or	U.S. Air Force 1990
	in contact with acids; corrosive to	EM Industries 1987
	aluminum. Reacts with alkali metals.	
Flammability	Not combustible	U.S. Air Force 1990
Flash Point	Not combustible	U.S. Air Force 1990
Dissociation Constant	No data	
Henry's Law Constant	No data	
Molecular Diffusivity Coefficient	No data	
Air Diffusivity Coefficient	No data	
Fish Bioconcentration Factor	10-100 for copper	ATSDR 1990b
Shellfish Bioconcentration Factor	30,000 for copper in oysters	ATSDR 1990b
Taste Threshold (copper in water)	2.6 ppm	ATSDR 1990b
Conversion Factors	Not applicable, associated with particulate material	

#### II. ENVIRONMENTAL FATE

#### A. Environmental Release

Copper (Cu) commonly exists in three valence states, Cu<sup>0</sup> (metal), Cu<sup>+</sup> (cuprous), and Cu<sup>++</sup> (cupric). It can also be oxidized to a Cu<sup>+++</sup> state, but there are no important industrial Cu<sup>+++</sup> chemicals, and Cu<sup>+++</sup> ions are rapidly reduced to Cu<sup>++</sup> in the environment (ATSDR 1990b). Cupric sulfate and cupric chloride are very soluble in water [143 and 706 g/L, respectively (U.S. EPA 1987a; ATSDR 1990b)] and, when dissolved, become sources of Cu<sup>++</sup> ions; cupro chloride is a source of Cu<sup>+</sup> ions in solution, but it has comparatively low water solubility [0.062 g/L (U.S. EPA 1987a)]. Ethylenediaminetetraacetate (EDTA) has the ability to chelate divalent metal ions such as Cu<sup>++</sup>. The release of Cu<sup>++</sup> from the Cu-EDTA complex depends on the concentration of other divalent metal ions in solution. Copper occurs naturally in the environment primarily as Cu<sup>++</sup> salts, oxides, and complexes; but Cu<sup>+</sup> compounds and metallic copper (Cu<sup>0</sup>) also occur naturally (U.S. EPA 1984a). Copper and its compounds are ubiquitous in nature as part of the earth's crust and are found in plants and animals (ATSDR 1990b). The average concentration of copper found in the earth's crust is about 50 ppm (ATSDR 1990b).

Releases to the air from natural sources primarily involve windblown dust; however, volcanoes, decaying vegetation, forest fires, and sea water spray also contribute (ATSDR 1990b). Anthropogenic sources include releases from copper smelting industries, iron and steel industries, coal burning power plants and fabricating operations involving copper (U.S. EPA 1984a). The mean concentration of airborne copper is 5-200 ng/m³, which is associated with particulate matter (ATSDR 1990b). Copper is also released to water from industrial and sewage treatment discharges and naturally from soil weathering. Most of this copper is adsorbed to particulate matter. Natural sources of copper account for about 68% of copper released to streams and waterways. Domestic wastewater is the largest anthropogenic source of copper released to water. Copper can enter the drinking water from the water distribution system and

can exceed 1.3 ppm when the pipes have not been flushed during a period of disuse. The total amount of copper released to water was estimated at 28,848,000,000 tons for 1976; this represents about 2.4% of the total amount copper released to the environment. The majority of copper is released to the land primarily from copper mines and mills and is in the form of insoluble sulfides or silicates. Other sources include sludge from sewage treatment plants, municipal refuse, waste from electroplating, iron and steel producers, and discarded copper-containing products (plumbing and wiring) (ATSDR 1990b).

In 1992, releases of copper to environmental media, as reported to the TRI by certain types of U.S. industries, totaled about 55,294,095 pounds of which 41,093,203 pounds were copper compounds and 14,200,892 pounds were metallic copper. Of these amounts, 6,329,997 pounds of copper compounds and 1,495,369 pounds of metallic copper (14.2%) were released to the atmosphere, 72,423 pounds of copper compounds and 41,474 pounds of metallic copper (0.2%) were released to surface water, 201,431 pounds of copper compounds and 16,736 pounds of metallic copper (0.4%) were released in underground injection sites, and 34,489,362 pounds of copper compounds and 12,647,313 pounds of metallic copper (85.2%) were released to land (TRI92 1994).

## **B.** Transport

- 1. <u>Air</u> Most of the copper in the air is in the form of particulate matter (dust) or is adsorbed to particulate matter. Larger particles (>5 μm) are removed by gravitational settling, smaller particles are removed by other forms of dry and wet deposition (ATSDR 1990b). Atmospheric copper resulting from combustion is associated with sub-micron particles that can remain in the troposphere for an estimated 7-30 days and may be carried long distances (ATSDR 1990b). In southern Ontario, Canada, the average copper concentration in rainwater was 1.57 ppb during 1982, and the average annual wet deposition of copper was 1.36 mg/m². The average annual wet deposition for both central and northern Ontario was 1.13 mg/m² (ATSDR 1990b).
- 2. Soil Most of the copper deposited in the soil is strongly adsorbed primarily to organic matter, carbonate minerals, clay minerals, and hydrous iron and manganese oxides. Movement through the soil is dependent on the presence of these substances, the pH, and other physical and chemical parameters. The greatest potential for leaching is seen in sandy soils with low pH (ATSDR 1990b). Laboratory experiments using controlled models and field experiments utilizing core samples have shown that very little copper moves through the soil. Core samples showed that some movement occurred as far as the 22.5-25 cm layer of soil, but little, if any, moved below this zone. The evidence indicates that hazardous amounts of copper should not leach into groundwater from sludge, even from sandy soils (ATSDR 1990b).
- 3. Water Copper in solution is present almost exclusively as the Cu<sup>++</sup> valence state (U.S. EPA 1987a). The Cu<sup>+</sup> ion is unstable in solution and disproportionates to Cu<sup>++</sup> and copper metal unless a stabilizing ligand is present (ATSDR 1990b). In sea water, Cu<sup>+</sup> was found to be more stable than in fresh water existing as CuClOH<sup>-</sup> ions. A photochemical reduction mechanism involving H<sub>2</sub>O<sub>2</sub> is thought to be partly responsible. The presence of Cu<sup>+</sup> is highest in the surface layer of seawater and can account for as much as 15% of the copper in seawater (ATSDR 1990b). Copper in the Cu<sup>++</sup> valence state forms compounds and complexes with a variety of organic and inorganic ligands binding to -NH<sub>2</sub>, -SH, and, to a lesser extent, -OH groups (ATSDR 1990b). The predominant form of copper in aqueous solution is dependent on the pH of the solution. Below pH 6, the cupric ion (Cu<sup>++</sup>)

predominates; copper complexes with carbonate usually predominate above pH 6 (U.S. EPA 1987a; ATSDR 1990b). The association of copper with organic or inorganic ligands also depends on the pH and on the CaCO<sub>3</sub> alkalinity. Rivers in the northwestern U.S. with a relatively high pH (7.0-8.5) and 24-219 ppm CaCO<sub>3</sub> were found to contain copper associated primarily with CO<sub>3</sub><sup>-</sup> and OH<sup>-</sup> ions. Under these conditions, copper can precipitate as malachite (Cu<sub>2</sub>(OH)<sub>2</sub>CO<sub>3</sub>). Copper was found to be largely associated with organic matter in lakes and rivers with a lower pH (4.6-6.3) and CaCO<sub>3</sub> concentration (1-30 ppm) such as found in southern Maine (ATSDR 1990b).

Most of the copper entering surface water is in the form of particulate matter, which settles out, precipitates, or adsorbs to organic matter, hydrous iron and manganese oxides, and clay; however, the predominating form can change with the amount of rain, pH, content of runoff, and the availability of ligands (ATSDR 1990b). The processes of complexation, adsorption and precipitation limit the concentration of copper (Cu<sup>++</sup>) to very low values in most natural waters (ATSDR 1990b). Copper discharged into a river upstream from the Chesapeake Bay was measured at 53 ppb. Copper associated with particulate material that were settleable solids accounted for 36 ppb. The copper concentration decreased rapidly downstream to 7 ppb 2-3 km from the pollution source. The copper concentration in the settlement, however, was 10 times the concentration in uncontaminated areas (ATSDR 1990b).

4. <u>Biota</u> — Calculations of the bioconcentration factor in fish for copper have ranged from 10 to 100; however, the majority of copper measurements in fish tissues under environmental conditions have indicated little, if any, bioconcentration. The copper content of fish muscle tissue taken from copper-contaminated lakes near Sudbury, Ontario were found to contain about the same level of copper as fish from uncontaminated areas (ATSDR 1990b). Filter feeding shellfish, especially oysters, however, were found to significantly concentrate copper with bioconcentration factors as high as 30,000 (ATSDR 1990b).

## CHEMICAL SUMMARY FOR DIETHYLENE GLYCOL MONOETHYL ETHER ACETATE

This chemical was identified by one or more suppliers as a bath ingredient for the conductive ink process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

### I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of diethylene glycol monoethyl ether acetate (DGEEA) are summarized below. In the body, glycol ether esters are apparently saponified (hydrolyzed) to the parent glycol ether and an organic acid. Systemic effects of the esters are typical of those of the corresponding parent glycol ethers (HSDB 1996), which for DGEEA, is diethylene glycol monoethyl ether (DGEE). Therefore, this report will also provide information on DGEE.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF DGEEA

Characteristic/Property	Data	Reference
CAS No.	112-15-2	
Common Synonyms	DGEEA; 2-(2-ethoxyethoxy)ethanol acetate;	Gingell et al. 1994
•	Carbitol® acetate	•
Molecular Formula	$C_8H_{16}O_4$	Gingell et al. 1994
Chemical Structure	C <sub>2</sub> H <sub>5</sub> OCH <sub>2</sub> CH <sub>2</sub> OCH <sub>2</sub> CH <sub>2</sub> OOCCH <sub>3</sub>	Gingell et al. 1994
Physical State	colorless liquid; hygroscopic	HSDB 1996
Molecular Weight	176.2	
Melting Point	-11°C, -25°C	Verschueren 1996
Boiling Point	217.4°C @ 760 mm Hg	Gingell et al. 1994
Water Solubility	miscible	HSDB 1996
Density	specific gravity (25/4°C), 1.01	Gingell et al. 1994
Vapor Density (air = 1)	6.07	Gingell et al. 1994
$K_{oc}$	not found	
Log K <sub>ow</sub>	not found	
Vapor Pressure	0.05 mm Hg @ 25°C	Gingell et al. 1994
Reactivity	not found	
Flammability	must be preheated before ignition	HSDB 1996
Flash Point	open cup, 225°F (107°C)	HSDB 1996
Dissociation Constant	not found	
Henry's Law Constant	not found	
Molecular Diffusivity Coefficient	not found	
Air Diffusivity Coefficient	not found	
Fish Bioconcentration Factor	not found	
Odor Threshold	50% recognition, 0.157 ppm	Verschueren 1996
	100% recognition, 0.263 ppm	
Conversion Factors	1 ppm $\approx 7.20 \text{ mg/m}^3 \text{ @ } 25^{\circ}\text{C}, 760 \text{ mm Hg}$	Gingell et al. 1994
	$1 \text{ mg/m}^3 \approx 0.1389 \text{ ppm}$	

#### II. ENVIRONMENTAL FATE

#### A. Environmental Release

No information was found in the secondary sources searched regarding the environmental release of DGEEA. The ester probably enters the environment as does its parent ether, DGEE, i.e., via effluents from sites where it is produced or used as a solvent and from other industries (Howard 1993). In a national survey of wastewater effluents, DGEE occurred in 5 of 21 industrial categories (Howard 1993). Average concentrations of DGEE in wastewater from various industries were as follows: 497 mg/L (iron and steel); 52,189 mg/L (printing and publishing); 175 mg/L (amusement and athletic goods); and 40 mg/L (pulp and paper) (Howard 1993). DGEE has also been found in

effluents from publicly-owned treatment works (Howard 1993). A drinking-water survey identified DGEE as a contaminant in 11 U.S. cities and 1 county (Howard 1993).

## **B.** Transport

The low vapor pressure of DGEEA (0.05 mm Hg [Gingell et al. 1994]) suggests that volatilization from soil or water will not be a significant transport mechanism for the chemical. DGEEA is miscible with water and may move through the soil, possibly to groundwater.

The parent ether, DGEE, is also miscible with water and has an estimated Henry's Law Constant of  $8.63 \times 10^{-10}$  atm-m³/mole at  $25 \,^{\circ}$ C (Howard 1993). This indicates that volatilization from natural bodies of water and moist soils should not be a significant fate process for the ether. The calculated  $K_{OC}$  value (20) for DGEE indicates that the chemical will be highly mobile in soil and should not partition from the water column to organic matter in sediments and suspended solids (Howard 1993).

## C. Transformation/Persistence

No information was found in the secondary sources searched regarding the transformation/persistence of DGEEA in the environment. However, inferences can be drawn regarding the fate of DGEEA, based on the following data for its parent ether, DGEE.

- 1. <u>Air</u> DGEE in ambient air exists mostly in the vapor phase (Howard 1993). The putative removal mechanisms for atmospheric DGEE are vapor phase reactions with photochemically produced hydroxyl radicals (Howard 1993). The estimated rate constant of 2.93 x 10<sup>-11</sup> cm<sup>3</sup>/molecule-sec @ 25°C for DGEE corresponds to a half-life of about 13 hours, assuming the atmospheric concentration of hydroxyl radicals is 5 x 10<sup>5</sup> per cm<sup>3</sup> (Howard 1993). Wet deposition of DGEE is limited by its short residence time (Howard 1993).
- 2. <u>Soil</u> The results of aqueous screening tests indicate that biodegradation is the most significant mechanism for the removal of DGEE from aerobic soil (see the results of screening tests in section II.C.3) (Howard 1993). Hydrolysis and direct photolysis are not important mechanisms for the removal of DGEE from soil (Howard 1993).
- 3. Water The results of aqueous screening tests indicate that biodegradation is the primary mechanism for the removal of DGEE from water (Howard 1993). After 16 days of acclimation, losses of 39.8% and 34.3% were recorded using an 8-hour Warburg test and a 5-day BOD (biochemical oxygen demand) test, respectively (Howard 1993). In two assays conducted without acclimation, the BODT values after 20-day incubation periods were 48 and 87% (Howard 1993). Using the Zahn-Wellens screening method, a >90% loss of the original concentration of DGEE (400 ppm) occurred in 28 days (Howard 1993). DGEE should not undergo hydrolysis or direct photolysis in the aquatic environment (Howard 1993).
- 4. <u>Biota</u> The calculated log BCF (bioconcentration factor) of -0.34 for DGEE and its miscibility with water indicate that the chemical will not bioconcentrate in aquatic organisms (Howard 1993).

#### CHEMICAL SUMMARY FOR DIETHYLENE GLYCOL METHYL ETHER

This chemical was identified by one or more suppliers as a bath ingredient for the conductive ink process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

#### I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of diethylene glycol methyl ether are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF DIETHYLENE GLYCOL METHYL

Change A spirit in (Dramage to 1)			
Characteristic/Property	Data	Reference	
CAS No.	111-77-3		
Common Synonyms	2-(2-methoxyethoxy) ethanol, methyl	HSDB 1995	
	carbitol, MECB, Dowanol DM, DGME	CHEMFATE 1995	
Molecular Formula	$C_5H_{12}O_3$		
Chemical Structure	CH <sub>3</sub> OCH <sub>2</sub> OCH <sub>2</sub> CH <sub>2</sub> OH		
Physical State	colorless liquid	HSDB 1995	
Molecular Weight	120.15	CHEMFATE 1995	
Melting Point	<-84°C	HSDB 1995	
Boiling Point	193°C	HSDB 1995	
Water Solubility	completely miscible	U.S. EPA 1984b	
	$1 \times 10^6$ mg/L at $25^{\circ}$ C	CHEMFATE 1995	
Density	$d^{20/4}$ , 1.035	HSDB 1995	
Vapor Density $(air = 1)$	4.14	HSDB 1995	
$K_{OC}$	10	HSDB 1995	
Log K <sub>ow</sub>	-0.68 (calculated)	CHEMFATE 1995	
	-0.790.93	U.S. EPA 1984b	
Vapor Pressure	0.18 mm Hg at 25°C	CHEMFATE 1995	
Reactivity	can react with oxidizing materials	HSDB 1995	
Flammability	moderate when exposed to heat		
	or flame	HSDB 1995	
Flash Point	200°F (93°C)	HSDB 1995	
Dissociation Constant	no data		
Henry's Law Constant	$6.5 \times 10^{-10} \text{ atm-cm}^3/\text{mole at } 25^{\circ}\text{C}$	HSDB 1995	
Molecular Diffusivity Coefficient	no data		
Air Diffusivity Coefficient	no data		
Log Bioconcentration Factor	-0.75 (estimated)	HSDB 1995	
Odor Threshold	no data; mild, pleasant	HSDB 1995	
Conversion Factors	$1 \text{ ppm} = 4.91 \text{ mg/m}^3$		
	$1 \text{ mg/m}^3 = 0.204 \text{ ppm}$	HSDB 1995	

#### II. ENVIRONMENTAL FATE

#### A. Environmental Release

No information was found regarding the quantity of diethylene glycol methyl ether (DGME) released to the environment. The chemical has been identified as a contaminate in drinking water samples (concentrations not listed) from cities across the continental U.S. (HSDB 1995. An average concentration of 3571 mg/L was found in the wastewater from paint and ink industries (HSDB 1995).

#### **B.** Transport

Because of the high water solubility and low Henry's Law Constant, most of the DGME released to the environment should end up in aquatic environments. The low  $K_{\text{OC}}$  indicates that the chemical can leach into ground water from soils; volatilization from water and soils is not an

important transport process (HSDB 1995). Removal from the atmosphere in precipitation is possible (HSDB 1995).

- 1. <u>Air</u> DGME should not undergo direct photolysis. The reaction rate constant with hydroxyl radicals has been estimated to be 2.44 x 10<sup>-11</sup> cm<sup>3</sup>/molecule-sec and corresponds to an atmospheric half-life of about 16 hours (HSDB 1995).
- 2. <u>Soil</u> In general, biodegradation and leaching would be the most important removal processes for glycol ethers in soils (U.S. EPA 1984b).
- 3. <u>Water</u> DGME was degraded by 0, 21, and 66% after 5, 10, and 20 days respectively when settled waste water or sewage sludge was used as inoculum (HSDB 1995).
- Biota Based on the high water solubility and low estimated bioconcentration factor of DGME, the chemical would not be expected to bioconcentrate in aquatic animals (HSDB 1995).

#### CHEMICAL SUMMARY FOR DIETHYLENE GLYCOL N-BUTYL ETHER

This chemical was identified by one or more suppliers as a bath ingredient for the conductive ink process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

#### I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of diethylene glycol n-butyl ether are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF DIETHYLENE GLYCOL N-BUTYL ETHER

Characteristic/Property	Data	Reference
CAS No.	112-34-5	
Common Synonyms	diethylene glycol monobutyl ether;	
	butyl carbitol	Budavari et al. 1989
Molecular Formula	$C_8H_{18}O_3$	Budavari et al. 1989
Chemical Structure	HOCH <sub>2</sub> CH <sub>2</sub> OCH <sub>2</sub> CH <sub>2</sub> OC <sub>4</sub> H <sub>9</sub>	Budavari et al. 1989
Physical State	liquid	Budavari et al. 1989
Molecular Weight	162.22	Budavari et al. 1989
Melting Point	-68°C	Budavari et al. 1989
Boiling Point	230.4°C	Budavari et al. 1989
Water Solubility	1 x 10 <sup>6</sup> mg/L at 25°C	CHEMFATE 1995
Density	0.9536	Budavari et al. 1989
Vapor Density (air = 1)	5.58	Gingell et al. 1994
K <sub>OC</sub>	75 (calculated)	HSDB 1995
Log K <sub>ow</sub>	0.91 (calculated)	CHEMFATE 1995
Vapor Pressure	0.0219 mm Hg at 25°C	CHEMFATE 1995
Reactivity	non reactive;	
•	NFPA rating: 0.0	HSDB 1995
Flammability	must be heated	HSDB 1995
Flash Point	500°F	Gingell et al. 1994
Dissociation Constant	no data	-
Henry's Law Constant	$1.52 \times 10^{-9} \text{ atm-m}^3/ \text{ mole at } 25^{\circ}\text{C}$	HSDB 1995
Molecular Diffusivity Coefficient	no data	
Air Diffusivity Coefficient	no data	
Fish Bioconcentration Factor	2.88 (estimated)	HSDB 1995
Odor Threshold	practically odorless	Budavari et al. 1989
Conversion Factors	1 ppm = $6.63 \text{ mg/m}^3$	Gingell et al. 1994
	$1 \text{ mg/m}^3 = 0.15 \text{ ppm}$	-

### II. ENVIRONMENTAL FATE

#### A. Environmental Release

In 1993 as reported to the TRI by certain types of U.S. industries, environmental releases of all glycol ethers totaled 45.9 million pounds; diethylene glycol n-butyl ether is not reported separately (TRI93 1995). The chemical has been detected in the waste water effluents from industries at average concentrations ranging from 7 to 244 mg/L (HSDB 1995).

#### **B.** Transport

Because of its miscibility with water, diethylene glycol n-butyl ether will partition to the water column and be highly mobile in soils. In the atmosphere, the chemical may be removed by precipitation and dissolution in clouds (HSDB 1995).

- <u>Air</u> In the atmosphere, diethylene glycol n-butyl ether should exist almost entirely in the vapor phase. The estimated half-life for reaction with hydroxyl radical is 11 hours (HSDB 1995).
- 2. <u>Soil</u> Diethylene glycol n-butyl ether should partition to the water column of moist soils and volatilization will not be significant (HSDB 1995).
- 3. <u>Water</u> Diethylene glycol n-butyl ether is not expected to undergo hydrolysis and the Henry's Law Constant indicates that volatilization would be slow. However, aerobic biodegradation may be an important removal mechanism from aquatic systems (HSDB 1995). No other information was found.
- 4. <u>Biota</u> Based on the estimated bioconcentration factor of 2.88 (HSDB 1995), diethylene glycol n-butyl ether should not bioaccumulate in aquatic organisms.

## CHEMICAL SUMMARY FOR N,N-DIMETHYLFORMAMIDE

This chemical was identified by one or more suppliers as a bath ingredient for the electroless copper process. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online data bases, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

#### I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of *N*,*N*-dimethylformamide are summarized below.

## CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF N,N-DIMETHYLFORMAMIDE

Characteristic/Property	Data	Reference
CAS No.	68-12-1	
Common Synonyms	DMF; DMFA; dimethylformamide; N,N-dimethylmethanamide;	IARC 1989
	<i>N</i> -formyldimethylamine	
Molecular Formula	C <sub>3</sub> H <sub>7</sub> NO	Budavari et al. 1989
Chemical Structure	HCON(CH <sub>3</sub> ) <sub>2</sub>	Budavari et al. 1989
Physical State	colorless to slightly yellow liquid	Budavari et al. 1989
Molecular Weight	73.09	Budavari et al. 1989
Melting Point	-61 °C	Budavari et al. 1989
Boiling Point	153°C @ 760 mm Hg	Budavari et al. 1989
Water Solubility	miscible with water	Budavari et al. 1989
Density	0.9445 @ 25/4°C	Budavari et al. 1989
Vapor Density (air = 1)	2.51	Verschueren 1983
K <sub>oc</sub>	7 (calculated)	HSDB 1996
Log K <sub>ow</sub>	-1.01	CHEMFATE 1996
Vapor Pressure	3.87 mm Hg @ 25°C	CHEMFATE 1996
Reactivity	can react vigorously with oxidizing agents,	HSDB 1996;
	halogenated hydrocarbons, and inorganic	Budavari et al. 1989
	nitrates; pH of $0.5$ molar soln. = $6.7$	
Flammability	combustible	HSDB 1996
Flash Point	67°C (153°F) (open cup)	Budavari et al. 1989
Dissociation Constant 0.3		CHEMFATE 1996
Air Diffusivity Constant	no data	
Molecular Diffusivity Constant	no data	
Henry's Law Constant	7.39 X 10E-8 atm-m <sup>3</sup> /mole @ 25°C	HSDB 1996
Fish Bioconcentration Factor	-1.01 (log; calculated)	HSDB 1996
Odor Threshold	0.14 mg/m³ (nonperception);	
	0.88 mg/m³ (perception); fishy odor	Verschueren 1983
Conversion Factors	$1 \text{ ppm} = 3.04 \text{ mg/m}^3$	
	$1 \text{ mg/m}^3 = 0.33 \text{ ppm}$	Verschueren 1983

#### II. ENVIRONMENTAL FATE

## A. Environmental Release

*N,N*-Dimethylformamide is a widely used solvent for organic compounds where a low rate of evaporation is required. The chemical may be emitted to the environment by effluents from a variety of petrochemical industries (Howard 1993).

N,N-Dimethylformamide has been identified in the air over a hazardous waste site in Lowell, MA and a neighboring industry at concentrations of 2.18 and >50 ppb, respectively; in 1 of 63 industrial wastewater effluents (<10  $\mu$ g/L); and in waste effluent of a plastics manufacturer (28,378 ng/ $\mu$ L extract). The chemical was listed as a contaminant found in drinking water

samples in several U.S. cities, and in 1 of 204 samples in a national survey of surface waters (Howard 1993).

## **B.** Transport

Volatilization of *N*,*N*-dimethylformamide from land or water is not expected to be significant (Howard 1993). The complete water solubility suggests that the chemical can be removed from the atmosphere by rainfall. *N*,*N*-dimethyl-formamide is expected to be highly mobile in soils and will probably leach into groundwater (U.S. EPA 1986).

- 1. <u>Air</u> Based upon the vapor pressure (3.87 mm Hg @ 25°C), *N*,*N*-dimethyl-formamide is expected to exist almost entirely in the gaseous phase in the atmosphere. The vapor phase reaction of *N*,*N*-dimethylformamide with photochemically produced hydroxyl radicals is likely to be an important fate process. The rate constant for the vapor phase reaction with photochemically produced hydroxyl radicals is estimated to be 2.24 x 10<sup>-10</sup> cm<sup>3</sup>/molecule-sec at 25°C, which corresponds to an atmospheric half-life of about 2 hours (Howard 1993). In smog chamber studies, *N*,*N*-dimethylformamide was relatively nonreactive with regard to photochemical oxidant formation (U.S. EPA 1986).
- 2. Soil The calculated K<sub>OC</sub> of 7 indicates that N,N-dimethylformamide will be highly mobile in soils and the Henry's Law Constant (7.39 x 10E<sup>-8</sup> atm-m<sup>3</sup>/mole) suggests that volatilization from soils will not be important (Howard 1993). Aqueous screening and a river die-away test suggests that biodegradation of N,N-dimethylformamide in soil will be rapid (HSDB 1996). When wastewater containing 250 mg/L N,N-dimethylformamide was aerobically treated with activated sludge, 95% of the chemical was degraded in 18 hours (U.S. EPA 1986).
- 3. Water The estimated K<sub>OC</sub> (ranging in the high mobility class for soil) indicates that *N*,*N*-dimethylformamide will not partition from the water column to organic matter contained in the sediments and suspended solids. The Henry's Law Constant suggests that volatilization from environmental waters will not be important (Howard 1993). *N*,*N*-Dimethylformamide hydrolyzes slowly in neutral pH water, but hydrolysis is accelerated by acids and bases (U.S. EPA 1986). *N*,*N*-Dimethylformamide can be biodegraded by activated sludge, although an acclimation period is usually required. River die-away data suggest that the biodegradation of the chemical should be rapid (Howard 1993).
- 4. <u>Biota</u> The bioconcentration factor of -1.01 (log) indicates that *N*,*N*-dimethyl-formamide will not bioconcentrate in aquatic organisms (Howard 1993).

#### CHEMICAL SUMMARY FOR ETHANOLAMINE

This chemical was identified by one or more suppliers as a bath ingredient for the electroless copper, carbon, graphite, and tin-palladium processes. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

#### I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of ethanolamine are summarized below.

CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF ETHANOLAMINE

Characteristic/Property	Data	Reference
CAS No.	141-43-5	
Common Synonyms	2-amino-1-ethanol; monoethanolamine;	
•	2-hydroxyethylamine; beta-aminoethanol;	
	glycinol; MEA	HSDB 1995
Molecular Formula	$C_2H_7NO$	Budavari et al. 1989
Chemical Structure	HOCH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>	Benya and Harbison 1994
Physical State	viscous hygroscopic liquid	Budavari et al. 1989
Molecular Weight	61.08	Budavari et al. 1989
Melting Point	10.3°C	Budavari et al. 1989
Boiling Point	170.8°C @ 760 mm Hg	Budavari et al. 1989
Water Solubility	completely soluble	Benya and Harbison 1994 Density
	1.0117 @ 25/4°C	Budavari et al. 1989
Vapor Density ( $air = 1$ )	2.1	HSDB 1995
K <sub>oc</sub>	5	HSDB 1995
Log K <sub>ow</sub>	-1.31	CHEMFATE 1995
Vapor Pressure	0.26 mm Hg at 25°C	HSDB 1995
Reactivity	reacts with strong oxidizers, strong acids,	NIOSH 1994
	iron; may attack copper, brass, rubber;	
	pH = 12.1 (0.1 N aqueous solution);	Budavari et al. 1989
	single or double substitution of the amine	Benya and Harbison 1994
	group leads to formation of a variety of compounds	
Flammability	2 (liquid which must be moderately heated	
•	before ignition will occur)	HSDB 1995
Flash Point	85°C, closed cup; 93.33°C open cup	ACGIH 1991
Air Diffusion Coefficient	no data	
Dissociation Constant	9.4994	CHEMFATE 1995
Molecular Diffusivity Coefficient	no data	
Henry's Law Constant	$4xE-8$ atm-m <sup>3</sup> /mole @ $25^{\circ}C$	CHEMFATE 1995
Fish Bioconcentration Factor	<1 (calculated)	HSDB 1995
Odor Threshold	3-4 ppm	ACGIH 1991
Conversion Factors	$1 \text{ ppm} = 2.54 \text{ mg/m}^3;$	Verschueren 1983
	$1 \text{ mg/m}^3 = 0.39 \text{ ppm}$	

#### II. ENVIRONMENTAL FATE

#### A. Environmental Release

Ethanolamine is a colorless viscous liquid with an unpleasant, fishy, ammoniacal odor (Budavari et al. 1989; Grant 1986). It is released to the environment primarily from emissions and effluents from sites of industrial production or use, from disposal of consumer products containing ethanolamine such as cleaning products, and use of agricultural products in which it is used as a dispersing agent. Ethanolamine can also be released to the environment in urine. Ethanolamine was one of the primary amines identified in aerosol samples collected over the North Atlantic Ocean. Highest concentrations were found in samples taken near North America,

Bermuda, the Azores, and in the Arctic Circle, and low concentrations in the Gulf stream and in the equatorial North Atlantic (Gorzelska and Galloway 1990, as reported in TOXLINE).

## **B.** Transport

Ethanolamine is completely soluble in water (Benya and Harbison 1994), and if released to the soil, would not be expected to adsorb appreciably to organic material [calculated  $K_{OC} = 5$  (HSDB 1995)]. Ethanolamine has the potential to leach into groundwater. The volatilization of ethanolamine from water is believed to be negligible [Henry's Law constant = 4E-8 atm-m³/mole @ 25°C (CHEMFATE 1995)].

- 1. <u>Air</u> The dominant removal mechanism is expected to be reaction with photochemically generated hydroxyl radicals. The calculated half-life for ethanolamine vapor reacting with hydroxyl radicals is 11 hours. The complete water solubility of ethanolamine suggests that this compound may also be removed from the atmosphere in precipitation (HSDB 1995).
- 2. <u>Soil</u> If released to soil, ethanolamine is expected to biodegrade fairly rapidly following acclimation and to leach in soil. The half-life is on the order of days to weeks. Volatilization from soil surfaces is not expected to be an important removal process (HSDB 1995).
- 3. Water If released to water, ethanolamine is expected to undergo biodegradation. The half-life of this compound may range from a few days to a few weeks depending, in large part, on the degree of acclimation of the system. Bioconcentration in aquatic organisms, adsorption to suspended solids and sediments, and volatilization are not important removal processes (HSDB 1995). Tests utilizing settled sewage seed showed that 0%, 58.4%, or 75% of added compound was biodegraded after 5, 10, or 50 days, respectively. In a closed activated sludge system, 93.6% of the added chemical was biodegraded (CHEMFATE 1995).
- 4. <u>Biota</u> The bioconcentration factor of <1 (based on a log K<sub>ow</sub> of -1.31) and the complete water solubility of ethanolamine suggest that the compound does not bioconcentrate in aquatic organisms (HSDB 1995).